Guidelines for preparing a new entry file for SWIC

The spin wave models must be submitted in the form of SpinW (matlab.m) or Su(n)ny Suite (Jupyter notebook (. ipynb) or Julia script (.jl) input files. Examples are given below.

The input files need to contain the following information:

- **Chemical formula of the material (no subscripts).**
  Ex: NaMn3(VO4)3(OH) or Ba3NbFe3Si2O14

- **Name and email address of the person who prepared the file.**

- **Give the reference to the published article** that describes the model. The reference should contain the full list of authors, journal name, volume number, page, and year:
  Ex: W. Szuszkiewicz, E. Dynowska, B. Witkowska, B. Hennion
  Phys. Rev. B. 73, 104403 (2006)
  https://doi.org/10.1103/PhysRevB.73.104403

- **Experimental details for the reported INS data that includes the following:**
  - Was the sample a powder or single crystal?
  - What instrument(s) /facility was used for collecting the data?
  - What temperature and magnetic field was the data collected at?

- **Provide information about the magnetic ground state of the material.**
  - Does the material orders? What is the transition temperature?
  - What is the propagation vector (k) of the ordered structure?
  - Is there an MCIF file available in the MAGNGDATA, at Bilbao server? If yes, please provide a link to that entry. Otherwise, it would be appreciated if a reference to the article reporting the magnetic structure is included.

  Ex: The system orders to an antiferromagnetic state with k = (1/2, 0, 0) at T_N = 310 K.
  The MCIF of magnetic structure is available in MAGNDATA:
  http://webbdcrista1.ehu.es/magndata/index.php?this_label=0.800

- **Include additional noteworthy comments about the spin-Hamiltonian model.** Things to consider are:
  - Was the original model described using a different definition of the Hamiltonian than those of the SpinW or Su(n)ny (i.e. Scale factors ½ or 2). Are the values of exchange parameters or single ion anisotropy listed in the model different from those reported in the paper, to ensure a better match to the experiment data?
  - Does the data description require the treatment of spins as SU(N) coherent states?
  - Was there any renormalization to the spin value done in the model?
  - Are there unexplained features in the experimental spectrum?
  - Is the optimized magnetic structure consistent to the magnetic order determined experimentally?

-If the material exhibits multiple magnetic transitions, then it is useful to specify the temperature or magnetic field range where the spin-wave model is applicable.

- **Define the magnetic sublattice by providing full crystallographic information that includes:**

- The lattice parameters, the space-group symmetry, and the non-equivalent positions for magnetic ions with site multiplicity. Specify the Wyckoff site if possible.
- Indicate the valence state of magnetic ions, and the corresponding spin quantum number used in the spin-Hamiltonian.

Note that it is preferable that the spin-wave models are using the space-group symmetry to generate the equivalent magnetic ions, even if the assignment of the exchange interacting is later split by sub-indexed atoms. We also prefer to not store CIF files in this database. If your original file is using a CIF file, please make the necessary changes to include all the crystal information inside the SpinW or Sunny input file.

- It is useful to also **include the Hamiltonian formula** (in Latex) in a way that clearly reflects the nature of the exchange couplings, DM interactions, and anisotropy. It is preferable to keep the same notations as in the paper.

Ex: *\mathcal{H}=\sum\limits_{<i,j>,n=1,2,3}J_{n}S_i\cdot S_j+ D\sum \limits_{i} (S_i^z)^2 \cr*
J_{1} = 3.7~meV; J_{2} = -0.115~meV ; J_{3} = 0.492~meV; D = 0.044~meV

$$H = \sum_{<i,j>,n=1,2,3} J_n S_i \cdot S_j + D \sum_i (S_i^z)^2$$

$$J_1 = 3.7\ \text{meV};; J_2 = -0.115\ \text{meV}; J_3 = 0.492\ \text{meV}; D = 0.044\ \text{meV}$$

- **The SpinW or Sunny files should run without errors**. Specify the program versions to use.

- **Ensure that the optimized magnetic structure is consistent with that reported in literature.** A plot of the structure needs to be created. If the k-vector or spins direction is not as expected, please revise the Hamiltonian parameters.

- **The model should calculate and plot the spin-wave dispersion** along the high-symmetry directions of the lattice, including those shown in the publication. This is a good opportunity to verify that the model is reproducing well the plots shown in the paper. The labeling of the Brillouin high symmetry points is optional.

- **Regardless of the type of experimental data discussed in the paper, both single-crystal dispersions and powder averaged spectra need to be calculated**. The calculated powder spectrum needs to account for the magnetic form factor, and the energy rage needs to capture the entire bandwidth. Typically, a Q range that extends to 3.5-4 A-1 is sufficient to highlight the most important features.

Example of SpinW file, with all required information:

```
%% chemical formula of the material
%  MnTe

%% file prepared by O. Garlea (ORNL), 2023
% email: garleao@ornl.gov

%% publication reference:
% W. Szuszkiewicz, E. Dynowska, B. Witkowska, B. Hennion
% Phys. Rev. B. 73, 104403 (2006)
% https://doi.org/10.1103/PhysRevB.73.104403

%% Experimental information from the article
% modeling of single crystal data collected at T = 11 K and 0 Tesla.
% The system orders magnetically at T_N = 310 K.
% data measured using the 2T1 spectrometer at Laboratoire Léon Brillouin

%% comments about the determined magnetic order (if known):
% Collinear structure with #k=(0, 0, 0) and moments lying in the ab-plane.
% MCIF of magnetic structure is available in MAGNDATA (Bilbao server),
% http://webbdcrista1.ehu.es/magndata/index.php?this_label=0.800

%% comments about the published model:
% The values of exchange parameters displayed in the paper have been adjusted to account
for a different definition of the Hamiltonian.

%% Define the lattice parameters, the Space-group symmetry and give the non-equivalent
positions for magnetic ions.

mnte = spinw;
mnte.genlattice('lat_const',[4.1475,4.1475,6.71],'angled',[90,90,120],...
   'spgr','P 63/m m c');

mnte.addatom('label','MMn2','r',[0,0,0],'S',5/2,'color','r');
mnte.gencoupling('maxdistance',6);

%% The reported values of exchange interactions and anisotropies (in meV)

%%% Exchange parameters in meV, converted from
% J1=-21.5 K, J2=0.67 K, and J3=-2.87 K, D=-0.26K (easy plane anisotropy)
% in SpinW, energies conversions can be done using J = sw_converter(-21.5,'K','meV');
%%% Energies were scaled by factor 2x from the paper to match experimental data.

J1 = 3.698; % 1.849*2 %
J2 = -0.115; % -0.0576*2
J3 = 0.492; %0.247*2
D = 0.044;
```

```
mnte.addmatrix('label','J_1','value',J1,'color','blue');
mnte.addmatrix('label','J_2','value',J2,'color','yellow');
mnte.addmatrix('label','J_3','value',J3,'color','cyan');
mnte.addmatrix('label','D','value',diag([0 0 D]),'color','g');

%% assign the exchange couplings to corresponding crystal bonds

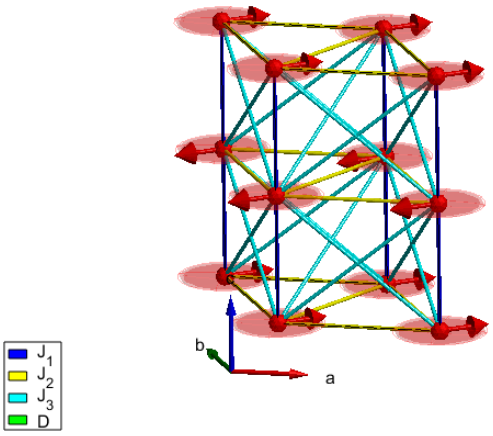
mnte.addcoupling('mat','J_1','bond',1);
mnte.addcoupling('mat','J_2','bond',2);
mnte.addcoupling('mat','J_3','bond',3);
mnte.addaniso('D');

%% define your initial magnetic structure

mnte.genmagstr('mode','helical','S',[1 -1; 0 0; 0 0],'k',[0,0,0],'n',[0,0,1],'nExt',[1 1 1]);
mnte.optmagsteep('nRun',1e4);

energ = mnte.energy

mnte.plot('range',[1,1,1],'cellmode','inside','atomlegend',false);
```



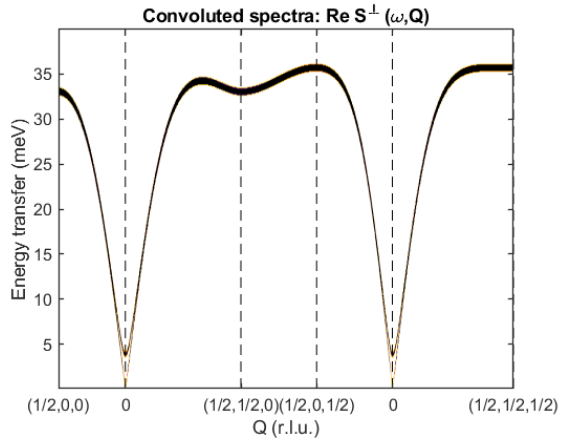

```
%% calculate and plot spin-wave dispersions along defined high-symmetry directions.

Q = {[0.5, 0.0, 0.0], [0,0,0], [0.5, 0.5, 0.0],[0.5, 0, 0.5],[0,0,0],[0.5, 0.5, 0.5],200};
Qlist={'(1/2,0,0)' '0' '(1/2,1/2,0)' '(1/2,0,1/2)' '0' '(1/2,1/2,1/2)'};

spec = mnte.spinwave(Q,'formfact',true);
spec = sw_neutron(spec);
spec = sw_egrid(spec,'component','Sperp','Evect',0:0.1:40);
spec = sw_omegasum(spec,'zeroint',1E-4);

figure();
sw_plotspec(spec,'mode','color','dashed',true,'dE',0.3,'axLim',[0 0.1],'qlabel',Qlist); colorbar
off;
%sw_plotspec(spec,'mode','disp','dashed',true,'axLim',[0 45],'colormap',[0 0
0],'qlabel',Qlist,'colorbar',false);
legend('MnTe','Location','northeast');
```

```
set(gca,'Layer','top','LineWidth',1,'Color','w','FontSize',12,'FontName', 'Arial')
```

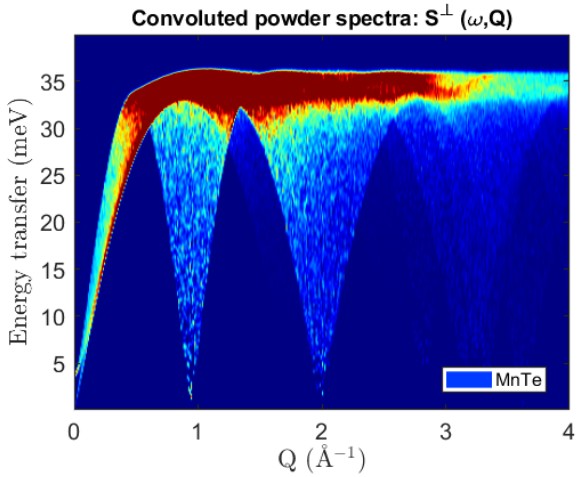



```
%% plot the powder averaged spin-wave spectrum

q=0:0.01:4;
de=0:0.05:40;

powspec = mnte.powspec(q,'evect',de,'nrand',1e3,'formfact',true);
figure();
sw_plotspec(powspec,'de',.5);

colormap(jet); colorbar off;
caxis([0,.12]);
legend('MnTe','Location','northeast');
ylabel('Energy transfer (meV)','fontsize',14,'interpreter','latex');
xlabel('Q (\AA$^{-1}$)','fontsize',14,'interpreter','latex');
set(gca,'Layer','top','LineWidth',1,'Color','w','FontSize',15,'FontName', 'Arial');
```



Example of Su(n)ny file, with all required information:

```
### Spin Wave model for MnTe
#  **Authors**: Ovi Garlea , garleao@ornl.gov<br>
# **Date**: Jan 23, 2024  (Sunny 0.5.8) <br>
# **Model reproduced from**: W. Szuszkiewicz, E. Dynowska, B. Witkowska, and B.
#  Hennion, Phys. Rev. B 73, 104403 (2006)._
https://doi.org/10.1103/PhysRevB.73.104403) <br>
#  **Experimental information from INS data**: parameters of the spin Hamitoninan
# were determined from modeling single crystal data
# INS data was measured using the 2T1 spectrometer at Laboratoire Léon Brillouin at T = 11
K and 0 Tesla. <br>
# The system orders magnetically at T_N = 310 K. <br>
# **Information on the determined magnetic structure**: Collinear structure with #k=(0,
0, 0) and
#  moments lying in the ab-plane. <br>
# MCIF of magnetic structure is available in MAGNDATA (Bilbao server) at
# http://webbdcrista1.ehu.es/magndata/index.php?this_label=0.800 <br>
# **Comments about the published model**: The values of exchange parameters
# displayed in the paper had to be doubled to account for a different definition of the
Hamiltonian.

using Sunny, GLMakie

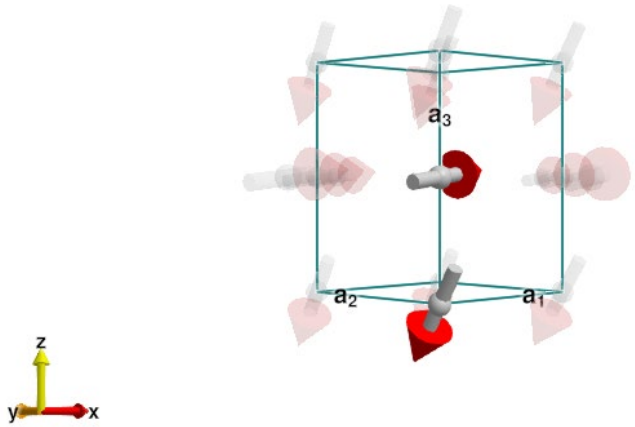
### System Definition for MnTe

lat_vecs    = lattice_vectors(4.1475, 4.1475, 6.71, 90, 90, 120)
positions  = [[0.0000, 0.0000, 0.0000]];
types = ["Mn"];
spgr   = 194;
MnTe   = Crystal(lat_vecs, positions, spgr; types, setting="1");
print_symmetry_table(MnTe, 10.0)

view_crystal(MnTe)

# System with quantum spin S=5/2 constrained to the space of dipoles, and
# randomize it.

spininfo = [SpinInfo(1; S=5/2, g=2)]
formfactors = [FormFactor("Mn2")];
latsize = (1,1,1)
sys  = System(MnTe, latsize, spininfo, :dipole; seed=1)
randomize_spins!(sys)
plot_spins(sys; ghost_radius=6.0)
```



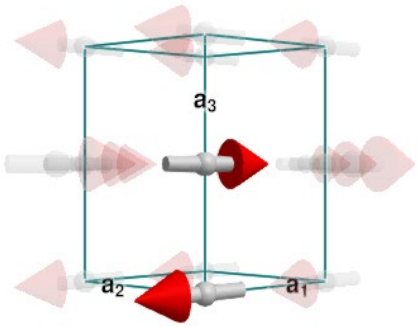
Define Exchange Interactions

```
J1 = 3.698 ;
J2 = -0.115 ;
J3 = 0.492 ;
D = 0.044 ;

set_exchange!(sys, J1, Bond(1, 2, [0,0,0])) # J1
set_exchange!(sys, J2, Bond(1, 1, [1,0,0])) # J2
set_exchange!(sys, J3, Bond(1, 2, [1,0,0])) # J3
#S = spin_matrices(5/2)
set_onsite_coupling!(sys, S -> D*S[3]^2, 1)
```

Plotting the spins confirms the expected Néel order.

```
randomize_spins!(sys)
minimize_energy!(sys)
plot_spins(sys; ghost_radius=6.0)
```



 # Dynamical Spin Structure Factor from Spin Wave Theory at T = 0 K

The $S(**q**,ω)$ is estimated with `SpinWaveTheory` and `intensity_formula`.
A Lorentzian broadening is applied to the calculation.

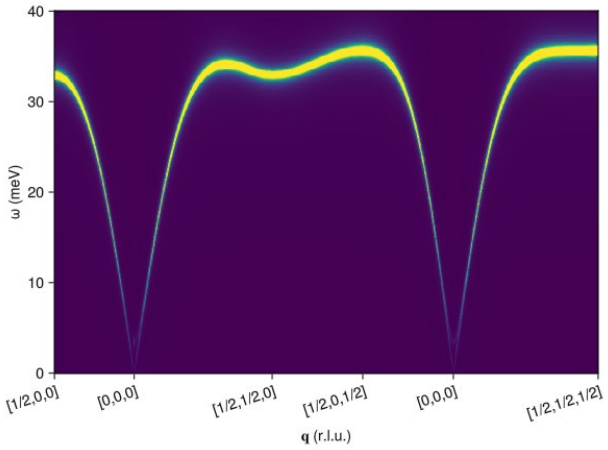
```
# The effect of `FormFactor` for Mn(2+) in intensity is also taken into account.

swt_mnte    = SpinWaveTheory(sys)
η      = 0.3 # (meV)
kernel  = lorentzian(η)
formula = intensity_formula(swt_mnte, :perp; kernel, formfactors)

# The spin wave dispersions from a "single crystal" along high-symmetry directions are
calculated below. <br>
# The `intensities_broadened` function collects intensities along this path.

Qpoints = [[0.5, 0.0, 0.0], [0,0,0], [0.5, 0.5, 0.0],[0.5, 0, 0.5],[0,0,0],[0.5, 0.5, 0.5]]
path, xticks = reciprocal_space_path(MnTe, Qpoints, 300)
energies = collect(0:0.1:40)
int = intensities_broadened(swt_mnte, path, energies, formula)

fig = Figure()
ax = Axis(fig[1,1]; aspect=1.5, ylabel="ω (meV)", xlabel="q (r.l.u.)",
        xticks, xticklabelrotation=π/10)
heatmap!(ax, 1:size(int, 1), energies, int, colormap=(:viridis),colorrange = (0, 0.3))
fig
```




```
# The powder averaged spectrum is calculated using the function
# `reciprocal_space_shell` to sample `n` wavevectors on a sphere of a given radius # (in
inverse angstroms).

radii = 0.01:0.02:4 # (1/Å)
output = zeros(Float64, length(radii), length(energies))
for (i, radius) in enumerate(radii)
   n = 1e3
   qs = reciprocal_space_shell(MnTe, radius, n)
   int = intensities_broadened(swt_mnte, qs, energies, formula)
   output[i, :] = sum(int, dims=1) / size(int, 1)
end
```

```
fig = Figure(fontsize=18)
ax = Axis(fig[1,1]; xlabel="|Q| (Å⁻¹)", ylabel="Energy transfer (meV)",title
=L"\text{Powder~averaged~spectrum~of~}MnTe")
heatmap!(ax, radii, energies, output, colormap=:jet, colorrange = (0, 0.3))
fig
```

